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ON THE SOLUTION OF A CERTAIN LINEAR LEAST SQUARES FIT PROBLEM.(U)
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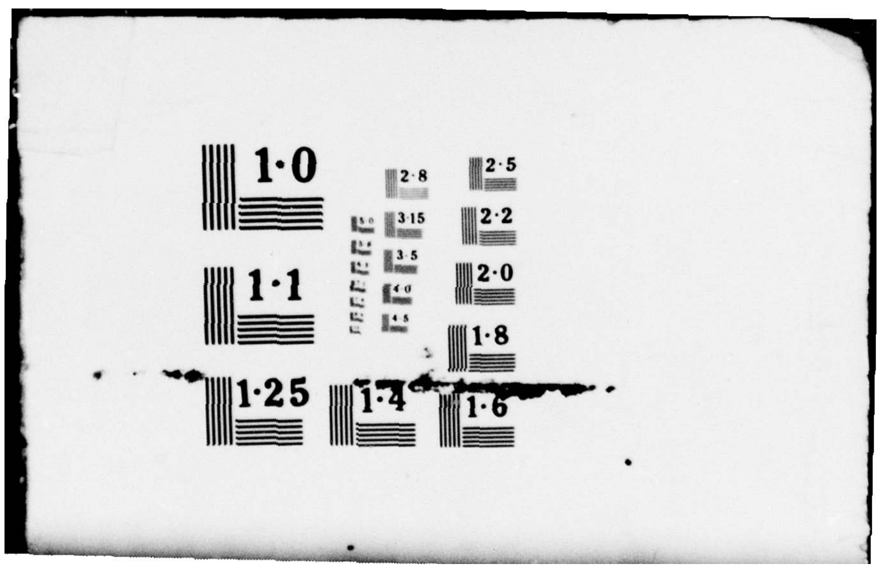
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DAVID W. TAYLOR NAVAL SHIP RESEARCH AND DEVELOPMENT CENTER

Bethesda, Md. 20084

DTNSRDC/CMLD-79/07

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ON THE SOLUTION OF A CERTAIN LINEAR LEAST SQUARES FIT PROBLEM

Donald A. Gignac

COMPUTATION, MATHEMATICS, AND LOGISTICS DEPARTMENT

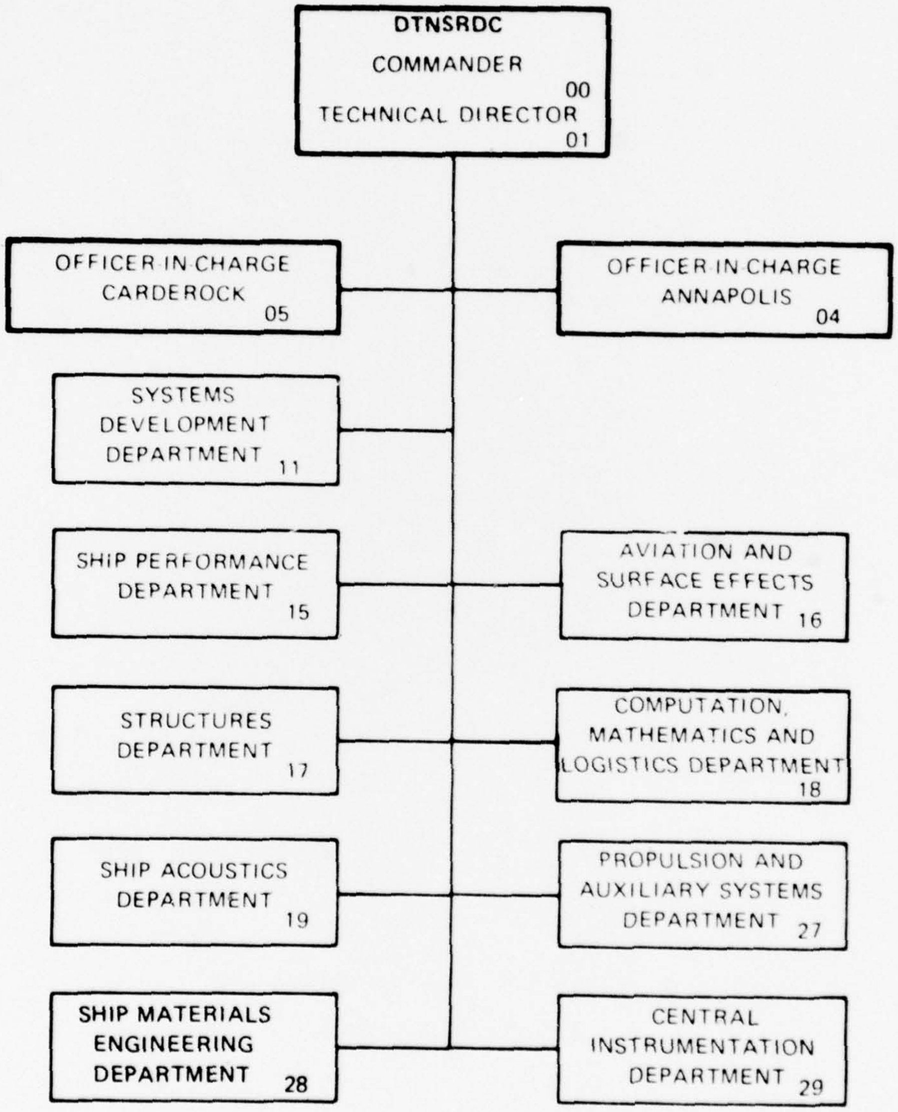
DEPARTMENTAL REPORT

June 1979

DTNSRDC/CMLD-79/07

ON THE SOLUTION OF A CERTAIN LINEAR LEAST SQUARES FIT PROBLEM

MAJOR DTNSRDC ORGANIZATIONAL COMPONENTS



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This report investigates the difficulties encountered with respect to a certain linear least squares fit problem which arises in the field of holographic interferometry. It was found that the addition of another variable to the equations of this linear least squares fit problem explained these difficulties and provided consistent results. This report also demonstrates the usefulness of Stewart's recently published perturbation bounds for the purpose of error bounding.

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ABSTRACT

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INTRODUCTION

Recently Dr. Surendra K. Dhir (Head, Numerical Structural Mechanics Branch, Code 1844) called the author's attention to difficulties arising from a linear least squares fit problem involving holographic displacement measurements.[1*] In the problem described, it is desired to fit a polynomial of the form $w = ax + by + cz$ by a set of experimentally obtained data points (w_i, a_i, b_i, c_i), $i=1,\ldots,n$; but under certain circumstances the polynomial would have to be set up in a differenced form, i.e.,

$$w_{i+1}-w_i = (a_{i+1}-a_i)x + (b_{i+1}-b_i)y + (c_{i+1}-c_i)z \qquad i=1,\ldots,n-1$$

Although the polynomial can be fitted to this "differenced" data, the relationship between this "differenced" problem and the original problem is neither apparent nor simple.

One possible approach is to regard the two least squares fit problems as perturbations of one another (after adding a redundant equation to the

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* A complete listing of references is given on page 21.

"differenced" system). It was with this approach in mind that Dr. Elizabeth H. Cuthill (Assistant for Numerical Analysis, Code 1805) suggested investigation of Stewart's recently published perturbation bounds for the linear least squares fit problem.[2] These bounds were found to be very useful indeed. This report documents their application to the problem in holographic interferometry.

STEWART'S PERTURBATION BOUNDS

Let A be an m x n real matrix of rank r. It is possible to find orthogonal matrices U and V of orders m and n, respectively, such that

$$U^T AV = \left(\begin{array}{cccc|c} \sigma_1 & & & & \\ & \sigma_2 & & & 0 \\ & & \ddots & & \\ & & & \sigma_r & \\ \hline & & 0 & & 0 \end{array}\right)$$

where $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_r > 0$. (It will be remembered that an orthogonal matrix U is a real matrix whose transpose U^T is its inverse.) The product $U^T AV$ is referred to as the singular value decomposition reduced or standard form of A. The σ_i, i=1,...r are called the singular values of A. The product

$$V \left(\begin{array}{cccc|c} 1/\sigma_1 & & & & \\ & 1/\sigma_2 & & & 0 \\ & & \ddots & & \\ & & & 1/\sigma_r & \\ \hline & & 0 & & 0 \end{array}\right) U^T$$

is called the pseudo-inverse of A, written A^T. The pseudo-inverse has many of the properties of the inverse of a square matrix. It is, in fact, a generalization of the concept of a matrix inverse. For more information on these topics, the reader is referred to Stewart.[3]

The formulas for Stewart's perturbation bounds require that A has been reduced to the singular value decomposition standard form. This

reduction involves no loss of generality since any m x n linear least square fit problem $Ax = b$ and any of its perturbations $(A+E)(x+h) = b+k$ can be reduced to this required form by the respective transformations

$$(U^T AV)(V^T x) = U^T b$$

$$(U^T AV+U^T EV)(V^T x+V^T h) = U^T b+U^T k$$

For the purpose of our problem we shall also assume that the columns of A are linearly independent and that the first n rows of A are also linearly independent.

Let the linear least squares fit problem $A(x+h)=b+k$ result from a perturbation of the right-hand side of $Ax = b$. Define κ as $\|A\|_2 \|A^\dagger\|_2$* and η as $\|b_1\|_2 / \|A\|_2 \|x\|_2$ where b_1 is the sub-vector of the first n components of b. Define k_1 similarly. Then Stewart provides the perturbation bound

$$\|h\|_2 / \|x\|_2 \leq \kappa\eta \|k_1\|_2 / \|b_1\|_2 \qquad \text{(Inequality 1)}$$

Next let the linear least squares fit problem $(A+E)x = b$ result from a perturbation of the coefficient matrix of $Ax = b$. Define $\bar{\kappa}$ as $\|A\|_2 \|B_{11}^{-1}\|_2$ where B_{11}^{-1} is the inverse of the n^{th} order principal submatrix of A+E. Let E_{11} be the n^{th} order principal submatrix of E and let E_{21} be the $(m-n) \times n$ submatrix of E below E_{11}. Define η and b_1 as before.

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* The reader is no doubt familiar with the concept of the norm of a vector x, written $\|x\|$, and defined by

$$\|x\| = \sqrt{\sum_{i=1}^{n} x_i^2}$$

where the x_i are the components of the vector x. Since there are several norms defined for vectors, let us be more precise and refer to the above norm as $\|x\|_2$. For A, an m x n real matrix, $\|A\|_2$ is defined to be σ_1, the largest singular value of A. It can be shown that $\|x\|_2 = \|Vx\|_2$ and $\|A\|_2 = \|U^T A V\|_2$ where U and V are unitary matrices. Accordingly this norm (along with others) is said to be unitarily invariant. For more information on norms and their properties the reader is referred to Stewart.[3]

Let b_2 be the m-n subvector of b below b_1. Then Stewart obtains the perturbation bound

$$\frac{\|h\|_2}{\|x\|_2} \le \bar{\kappa}\,\frac{\|E_{11}\|_2}{\|A\|_2} + \bar{\kappa}^2\,\frac{\|E_{21}\|_2}{\|A\|_2}\left(\eta\,\frac{\|b_2\|_2}{\|b_1\|_2} + \frac{\|E_{21}\|_2}{\|A\|_2}\right) \qquad \text{(Inequality 2)}$$

Define the real valued matrix function

$$\psi(F) = \frac{\|F\|_2}{(1+\|F\|_2^2)^{1/2}}$$

Stewart bounds the last term of Inequality 2 and obtains another perturbation bound

$$\frac{\|h\|_2}{\|x\|_2} \le \bar{\kappa}\,\frac{\|E_{11}\|_2}{\|A\|_2} + \bar{\kappa}\,\eta\,\frac{\|b_2\|_2}{\|b_1\|_2}\,\psi\left(\frac{\bar{\kappa}\,E_{21}}{\|A\|_2}\right) \qquad \text{(Inequality 3)}$$

Clearly these three inequalities can be used to provide "worst possible case" bounds for a given least square fit problem $Ax = b$. In the case of Inequality 1 one needs only to provide some upper bound for $\|k_1\|_2$ to obtain such a bound for $\|h\|_2 / \|x\|_2$ when only the right-hand side b is perturbed. As regards Inequalities 2 and 3 one must provide upper bounds for $\|E_{11}\|$ and $\|E_{21}\|$ to obtain similar worst possible case bounds for $\|h\|_2/\|x\|_2$ when only A is perturbed. The reader is reminded that

$$\|(A_{11}+E_{11})^{-1}\|_2 \le \frac{\|A_{11}^{-1}\|_2}{1 - \|A_{11}^{-1}\|_2\,\|E_{11}\|_2}$$

(see Wilkinson,[4] p. 92) if $\|A_{11}^{-1}\|_2\|E_{11}\|_2 < 1$. In Inequality 3 the function ψ may be bounded from above by 1.0.

THE TESTS

We shall refer to the 7 x 3 linear least squares fit problem $Ax = b$ where

$$A = \begin{matrix} -.21458051E+00 & -.59223911E+00 & -.18537080E+01 \\ -.35869262E+00 & -.54449323E+00 & -.18176699E+01 \\ -.22761852E+00 & -.47379546E+00 & -.18959881E+01 \\ -.30491734E+00 & -.45507956E+00 & -.18743727E+01 \\ -.37405904E+00 & -.43714104E+00 & -.18487759E+01 \\ -.23612950E+00 & -.35108814E+00 & -.19235878E+01 \\ -.38382191E+00 & -.32889374E+00 & -.18685387E+01 \end{matrix}$$

and

$$b = \begin{matrix} .36055440E-03 \\ .35650322E-03 \\ .35852881E-03 \\ .35650322E-03 \\ .35447764E-03 \\ .35650322E-03 \\ .35245205E-03 \end{matrix}$$

as the "original" problem. It is estimated that the elements of the columns of A and b are subject to uncertainties of 5%, 11%, 2%, and 5%, respectively.

We define the "differenced" 7 x 3 linear least squares fit problem thus: for i = 1,...,6 subtract the i^{th} equation from the $i+1^{st}$ equation of the original problem; the seventh equation of the differenced problem is the difference of the first and seventh equations of the original problem. We define the "augmented" 7 x 4 linear least squares fit problem merely by adding a fourth column of 1.0's to the coefficient matrix of the original problem and another unknown x_4 to the solution vector. Now solve this augmented problem for the value of x_4, take the original 7 x 3 linear least squares fit problem $Ax = b$ and subtract the value of x_4 from the right-hand side b of the original problem. We shall refer to the resulting 7 x 3 linear least squares fit problem as the "modified" problem.

These linear least square fit problems were perturbed ten times each. The ratio of the norm of the solution perturbation to the solution norm was computed along with their bounds provided by Inequalities 1 through 3. These results are compared in Tables 1-5 for perturbations* of either or

* The perturbations in Table 5 were reduced by a factor of 10 to meet the condition $\|A_{11}^{-1}\| \, \|E_{11}\| < 1$ for the approximation of $\|(A_{11} + E_{11})^{-1}\|_2$.

TABLE 1 - INEQUALITY 1 RESULTS

Perturbation	Original Problem			Differenced Problem			Augmented Problem		
	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 1 Bound	Worst Possible Bound 1	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 1 Bound	Worst Possible Bound 1	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 1 Bound	Worst Possible Bound 1
1	0.162	0.425	1.426	0.409	0.555	1.714	3.482	8.377	25.538
2	0.307	0.349	1.437	0.300	0.496	1.728	3.550	7.198	25.741
3	0.202	0.280	1.438	0.347	0.729	1.738	2.884	5.785	25.760
4	0.333	0.371	1.449	0.239	0.852	1.751	2.951	7.285	25.962
5	0.305	0.417	1.450	0.286	1.116	1.761	2.288	7.811	25.984
6	0.193	0.238	1.451	0.214	0.241	1.725	2.227	4.803	26.001
7	0.175	0.251	1.442	0.377	0.497	1.732	2.655	5.230	25.841
8	0.132	0.184	1.443	0.117	0.609	1.742	5.152	6.115	25.856
9	0.181	0.310	1.434	0.407	0.926	1.741	3.092	6.355	25.695
10	0.310	0.339	1.446	0.300	1.032	1.754	3.160	6.844	25.897

TABLE 2 - INEQUALITIES 2 AND 3 RESULTS

Perturbation	Original Problem			Differenced Problem			Modified Problem		
	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound
1	0.090	0.420	0.201	0.326	1.016	0.769	0.098	0.401	0.184
2	0.181	0.534	0.300	0.424	1.520	0.999	0.172	0.514	0.282
3	0.068	0.281	0.143	0.412	1.382	1.023	0.057	0.266	0.129
4	0.152	0.352	0.192	0.511	1.745	1.245	0.085	0.336	0.178
5	0.190	0.578	0.274	0.580	2.424	1.523	0.167	0.556	0.255
6	0.071	0.411	0.175	0.406	2.043	1.589	0.021	0.392	0.159
7	0.091	0.408	0.213	0.673	2.659	1.896	0.061	0.391	0.197
8	0.248	0.787	0.383	0.563	3.048	1.988	0.167	0.759	0.360
9	0.061	0.428	0.127	0.543	4.166	2.562	0.105	0.406	0.107
10	0.155	0.500	0.208	0.514	3.220	2.261	0.086	0.478	0.189

TABLE 3 - INEQUALITIES 1, 2, AND 3 RESULTS (JOINT VARIATION)

Perturbation	Original Problem			Differenced Problem		
	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequalities 1+2 Bound	Inequalities 1+3 Bound	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequalities 1+2 Bound	Inequalities 1+3 Bound
1	0.327	0.845	0.626	0.716	1.571	1.324
2	0.549	0.883	0.649	0.672	2.016	1.495
3	0.260	0.561	0.423	0.695	2.111	1.752
4	0.482	0.723	0.563	0.661	2.597	2.097
5	0.417	0.995	0.691	0.841	3.540	2.639
6	0.236	0.649	0.413	0.604	2.284	1.830
7	0.159	0.659	0.785	1.019	3.156	2.393
8	0.247	0.971	0.567	0.608	3.657	2.597
9	0.263	0.738	0.437	0.652	5.092	3.488
10	0.489	0.839	0.547	0.662	4.252	3.293

TABLE 4 - RESULTS ILLUSTRATIVE OF THE EFFECT OF THE FOURTH PARAMETER IN THE MODELING OF THE PROBLEM

Perturbation	Augmented Problem-- All Four Columns of a Perturbed			Augmented Problem-- First Three Columns of a Perturbed			Modified Problem-- Joint Variation			
	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|x\|\|_2}$	*Inequality* 1 Bound	*Inequality* 2 Bound	*Inequality* 3 Bound
1	1.033	55.454	3.802	0.234	854.805	12.382	6.489	164.686	0.401	0.184
2	0.974	1086.539	16.866	0.120	2270.770	30.324	7.305	166.113	0.514	0.282
3	0.907	17.133	1.961	0.066	94.114	3.193	6.357	166.241	0.266	0.129
4	0.976	25.356	2.402	0.076	38.646	2.852	7.100	167.669	0.336	0.178
5	1.006	14.791	1.795	0.189	7.000	6.996	6.879	167.804	0.556	0.255
6	0.839	32.004	2.228	0.048	72.742	3.438	6.331	167.940	0.392	0.159
7	0.914	8.517	1.816	0.119	2473.818	22.534	6.128	166.783	0.391	0.197
8	1.012	1191.792	16.300	0.168	140.175	6.585	6.329	166.917	0.760	0.360
9	1.006	36.107	1.741	0.063	44.546	2.479	6.353	165.765	0.406	0.107
10	1.002	142.086	3.737	0.306	341.516	6.784	7.113	167.192	0.478	0.189

TABLE 5 - UPPER BOUNDS TO INEQUALITIES 2 AND 3 BOUNDS

Perturbation	Original Problem			Differenced Problem			Modified Problem		
	Worst Possible Inequality 2 Bound = 0.2513 Worst Possible Inequality 3 Bound = 0.2123			Worst Possible Inequality 2 Bound = 3.5122 Worst Possible Inequality 3 Bound = 2.4646			Worst Possible Inequality 2 Bound = 0.2418 Worst Possible Inequality 3 Bound = 0.2028		
	$\frac{\|\|h\|\|_2}{\|\|\mathbf{x}\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|\mathbf{x}\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound	$\frac{\|\|h\|\|_2}{\|\|\mathbf{x}\|\|_2}$	Inequality 2 Bound	Inequality 3 Bound
1	0.0082	0.0219	0.0197	0.0285	0.0740	0.0721	0.0094	0.0201	0.0180
2	0.0166	0.0313	0.0291	0.0384	0.1056	0.1014	0.0131	0.0294	0.0273
3	0.0069	0.0160	0.0146	0.0382	0.0963	0.0937	0.0044	0.0145	0.0132
4	0.0146	0.0210	0.0195	0.0480	0.1242	0.1204	0.0084	0.0195	0.0179
5	0.0189	0.0305	0.0276	0.0520	0.1665	0.1593	0.0176	0.0284	0.0254
6	0.0040	0.0217	0.0191	0.0379	0.1596	0.1561	0.0016	0.0197	0.0170
7	0.0096	0.0240	0.0219	0.0610	0.1908	0.1851	0.0046	0.0221	0.0201
8	0.0218	0.0390	0.0356	0.0590	0.2360	0.2261	0.0180	0.0367	0.0333
9	0.0061	0.0155	0.0127	0.0558	0.2514	0.2412	0.0064	0.0134	0.0106
10	0.0148	0.0242	0.0213	0.0499	0.2645	0.2553	0.0094	0.0220	0.0191

both the right- and left-hand sides of these problems. We shall comment on these results in the next section. These results were obtained by single precision computation on the CDC 6400 at DTNSRDC. Subroutines from the IMSL Library[5] were used to compute singular value decompositions, solve linear least squares fit problems, and generate random numbers.

Let

$$A' = \begin{pmatrix} -.21458043E{+}00 & -.61617945E{+}00 & -.18521478E{+}01 \\ -.36091016E{+}00 & -.52242982E{+}00 & -.18192539E{+}01 \\ -.21953501E{+}00 & -.52034141E{+}00 & -.18609241E{+}01 \\ -.31149031E{+}00 & -.41563715E{+}00 & -.18808611E{+}01 \\ -.36469258E{+}00 & -.43905926E{+}00 & -.18250381E{+}01 \\ -.23855953E{+}00 & -.32482739E{+}00 & -.19453948E{+}01 \\ -.38297324E{+}00 & -.33146348E{+}00 & -.18640814E{+}01 \end{pmatrix}$$

and

$$b' = \begin{pmatrix} .36055496E{-}03 \\ .34712449E{-}03 \\ .35893074E{-}03 \\ .34162634E{-}03 \\ .35680069E{-}03 \\ .34089129E{-}03 \\ .35576825E{-}03 \end{pmatrix}$$

be the perturbations of the A and b matrices defined previously. The solution of the original problem $Ax = b$ is

$$x \approx \begin{pmatrix} -.41300149E{-}04 \\ -.66551182E{-}04 \\ -.16793035E{-}03 \end{pmatrix}$$

The solution x' of the problem $Ax' = b$ (only b perturbed) is

$$x' \approx \begin{pmatrix} -.67766679E{-}04 \\ -.77162085E{-}04 \\ -.15851240E{-}03 \end{pmatrix}$$

The solution x'' of $A'x'' = b$ (only coefficient matrix perturbed) is

$$x'' \approx \begin{pmatrix} -.56582677E{-}04 \\ -.72542926E{-}04 \\ -.16455871E{-}03 \end{pmatrix}$$

The solution x''' of $A'x''' = b'$ (both b and coefficient matrix perturbed) is

$$x''' \approx \begin{pmatrix} -.88120583E{-}04 \\ -.10061679E{-}03 \\ -.15007406E{-}03 \end{pmatrix}$$

These results should prove useful as benchmark results for those who wish to run the problems published in this report.

OBSERVATIONS AND CONCLUSIONS

Let us begin by explaining the discrepancy between the solutions of the original and the differenced linear least squares fit problems. A system of m linear equations in n unknowns $Ax = b$ is said to be consistent if there exists a solution vector x which satisfies each equation of this system exactly. It is obvious from the rules of algebraic manipulation that any solution of a consistent system is likewise a solution of its differenced system. If $Ax = b$ is inconsistent, we define the linear least squares fit "solution" to be that real vector x which minimizes the norm of the residual vector $r = Ax - b$. Thus it is merely a notational convenience to write an inconsistent linear least squares fit problem as $Ax = b$, since equality obtains only when we include the residual vector r thus

$$Ax = b + r$$

If we construct the differenced system by subtracting the equations of this last system from one another, we can see that the residual vector r' for x with respect to the differenced system is

$$r' = \begin{pmatrix} r_1 - r_2 \\ r_2 - r_3 \\ \vdots \\ r_n - r_1 \end{pmatrix}$$

In general r' is not the residual vector of minimum norm for the differenced system and hence x is not the least squares fit solution for the differenced system.

Next let us consider the modeling of the original 7 x 3 problem. If we include an extra variable k in each equation of the original system (thus obtaining the 7 x 4 augmented system), we find that the first three unknowns of the augmented system least squares fit solution do not agree at all with the least squares fit solution of the original system. Rather,

they coincide with the least squares fit solution of the 7×3 system whose coefficient matrix is A but whose right-hand side is diminished by the value of k (modified system). Clearly this fourth unknown k is crucial.

Finally, this investigation has demonstrated the value of using Stewart's perturbation bounds in the error analysis of the linear least squares fit problem. In particular the Inequality 1 estimates seem to bound $\|h\|_2/\|x\|_2$ quite nicely when only b is perturbed. In fact these Inequality 1 bounds are roughly a third of the worst possible error estimate afforded by Inequality 1. As might be expected the Inequalities 2 and 3 estimates do not bound $\|h\|_2/\|x\|_2$ when A is perturbed as closely as the Inequality 1 estimates do for perturbed b. However at worst the Inequalities 2 and 3 estimates appear to be not greater than eight times $\|h\|_2/\|x\|_2$. Usually the Inequality 3 bounds are "sharper" (closer) than the Inequality 2 bounds, although this is not always the case. These Inequalities 2 and 3 bounds are roughly a tenth of the worst possible error estimates provided by Inequalities 2 and 3, respectively.

So far all results obtained indicate that the errors from a joint perturbation of A and b are roughly the sum of the respective errors and hence may be bounded by the sum of the bounds provided by Inequalities 1 and 2 or 1 and 3.

PROGRAMS

The following programs were used to obtain some of the results published in this report. The reader is reminded of the special row and column rank conditions holding for this problem. In particular, the procedure for obtaining an $m \times m$ unitary matrix U' from the $m \times m$ unitary matrix U output from the LSVALR subroutine works only under these conditions. (The last m-n columns of the $m \times m$ identity matrix I are annexed to the $m \times m$ matrix U. U' is obtained by orthogonalizing these m columns using Gram-Schmidt algorithm. Of course, this procedure can be generalized by modifying it with suitable before and after permutations.)

```
      PROGRAM SKDPROB(OUTPUT,TAPE6=OUTPUT)
C
      DIMENSION A(7),B(7),C(7),AA(7,3),BB(7),R(7),WKAREA(99),X(7),Y(7),
     1 Z(7),XN(7),S(7),CC(7),CDOS(3,3),Q(7,3),H(7),V(7,7),G(7,3)
      DIMENSION TKK(3,3),BQ(3)
      DIMENSION T(7)
      DIMENSION QQ(7,3),QB(7),QC(7,7),QD(3,3),QE(3)
      DIMENSION QU(7,7),XKK(7),XK(7)
      DIMENSION QF(7)
      DIMENSION QP(7,3)
      DIMENSION E11(7,3),GG(7,3),GQ(7),GU(7,3),GV(3,3),GH(7,3),EL(7,3),
     1    QR(7,3),ET(7,3)
      DIMENSION E21(4,3)
      DIMENSION CF(7)
C
      DO 34 JQ=1,10
      IF (JQ.EQ.1) KQ=JQ
C
      XX=-5.165+6.1
      YY=-2.459-0.7
      ZZ=2.53-19.4
      X0=Y0=Z0=0.0
      R0=SQRT((XX-X0)*(XX-X0)+(YY-Y0)*(YY-Y0)+(ZZ-Z0)*(ZZ-Z0))
      X(1)=X(3)=X(6)=4.25
      X(2)=X(5)=X(7)=5.7
      X(4)=5.45
      Y(1)=Y(2)=1.875
      Y(3)=Y(4)=Y(5)=0.25
      Y(6)=Y(7)=-1.25
      Z(1)=Z(3)=Z(6)=-5.12
      Z(2)=Z(5)=Z(7)=-5.2
      Z(4)=-5.65
      DO 1 K=1,7
      R(K)=SQRT((XX-X(K))*(XX-X(K))+(YY-Y(K))*(YY-Y(K))+(ZZ-Z(K))*
     1            (ZZ-Z(K)))
      A(K)=(XX-X0)/R0+(XX-X(K))/R(K)
      B(K)=(YY-Y0)/R0+(YY-Y(K))/R(K)
    1 C(K)=(ZZ-Z0)/R0+(ZZ-Z(K))/R(K)
      XN(1)=17.8
      XN(2)=XN(4)=XN(6)=17.6
      XN(3)=17.7
      XN(5)=17.5
      XN(7)=17.4
      XLAMBDA=5145.0*3.937 E-09
      DO 47 I=1,7
      QQ(I,1)=A(I)
      QQ(I,2)=B(I)
      QQ(I,3)=C(I)
      QB(I)=XLAMBDA*XN(I)
      CF(I)=QB(I)
   47 QF(I)=QB(I)
      BNRM=SQRT(QB(1)**2+QB(2)**2+QB(3)**2+QB(4)**2+QB(5)**2+
     1 QB(6)**2+QB(7)**2)
      DO 48 J=1,3
      DO 48 I=1,7
      QR(I,J)=QQ(I,J)
   48 QP(I,J)=QQ(I,J)
```

```
      M=7
      N=3
      ISW=1
      WRITE(6,99) ((QQ(I,J),J=1,3),I=1,7)
   99 FORMAT(1X,2HQQ,3E16.8)
      CALL LSVALR(QQ,M,N,M,N,ISW,WKAREA,QE,QC,QD)
      ANRM=AMAX1(QE(1),QE(2),QE(3))
      XAPSI2=AMAX1(1.0/QE(1),1./QE(2),1./QE(3))
      WRITE(6,62) ((QC(I,J),J=1,3),I=1,7)
   62 FORMAT(1X,2HQC,3E16.7)
      CALL VCOMP(QC,QU,M,N)
      WRITE(6,63) ((QU(I,J),J=1,7),I=1,7)
   63 FORMAT(1X,2HQU,7E16.7)
      DO 15 I=1,7
      BB(I)=0.0
      DO 15 K=1,7
   15 BB(I)=BB(I)+QU(K,I)*QB(K)
      B1NRM=SQRT(BB(1)**2+BB(2)**2+BB(3)**2)
      B1NRM=SQRT(BB(1)**2+BB(2)**2+BB(3)**2)
      B2NM=SQRT(BB(4)**2+BB(5)**2+BB(6)**2+BB(7)**2)
      NB=1
      IDGT=8
      CALL LLSQAR(QP,QB,M,N,NB,M,M,IDGT,WKAREA,IER)
      WRITE(6,46) (I,QB(I),I=1,3)
   46 FORMAT(1X,2HQB,I10,E16.8)
      XSQD=QB(1)**2+QB(2)**2+QB(3)**2
      XNRM=SQRT(XSQD)
      HOLD=XNRM
      KQ=JQ
      CALL GGUB(KQ,7,T)
      DO 30 I=1,7
   30 A(I)=A(I)+(-1)**I*T(I)*.047*A(I)
      CALL GGUB(2*KQ,7,T)
      DO 31 I=1,7
   31 B(I)=B(I)-(-1)**I*T(I)*.113*B(I)
      CALL GGUB(3*KQ,7,T)
      DO 32 I=1,7
   32 C(I)=C(I)+(-1)**I*T(I)*.023*C(I)
      CALL GGUB(4*JQ,7,T)
      DO 33 I=1,7
   33 XN(I)=XN(I)-(-1)**I*T(I)*.05*XN(I)
      WRITE(6,212) (T(I),XN(I),I=1,7)
  212 FORMAT(1X,1HT,E16.8,2HXN,E16.8)
      XLAMBDA=5145.0*3.937 E-09
      DO 2 K=1,7
      BB(K)=XLAMBDA*XN(K)
      XKK(K)=BB(K)-CF(K)
      CC(K)=BB(K)
      AA(K,1)=A(K)
      AA(K,2)=B(K)
    2 AA(K,3)=C(K)
      DO 60 LL=1,3
      XK(LL)=0.0
      DO 60 K=1,7
   60 XK(LL)=XK(LL)+QC(K,LL)*XKK(K)
      XK2=XK(1)**2+XK(2)**2+XK(3)**2
      XK2=SQRT(XK2)
```

```
      RHS=(XAPSI2*XK2)/XNRM
      WRITE(6,65)RHS
   65 FORMAT(1X,4H RHS,E16.8)
      DO 83 I=1,7
      DO 83 J=1,3
      GG(I,J)=AA(I,J)
   83 Q(I,J)=AA(I,J)
      WRITE(6,50)
   50 FORMAT(1H1/1X,9HAA AND B3)
      WRITE(6,51)(AA(K,1),AA(K,2),AA(K,3),BB(K),K=1,7)
   51 FORMAT(1X,3E16.8,E20.8)

      DO 11 I=1,7
      DO 11 J=1,3
   11 ET(I,J)=QR(I,J)
      DO 68 I=1,7
      DO 68 J=1,3
      EL(I,J)=0.0
      GH(I,J)=0.0
      DO 68 K=1,3
      EL(I,J)=EL(I,J)+ET(I,K)*QD(K,J)
   68 GH(I,J)=GH(I,J)+GG(I,K)*QD(K,J)
      DO 69 I=1,7
      DO 69 J=1,3
      ET(I,J)=0.0
      GG(I,J)=0.0
      DO 69 K=1,7
      ET(I,J)=ET(I,J)+QU(K,I)*EL(K,J)
   69 GG(I,J)=GG(I,J)+QU(K,I)*GH(K,J)
      WRITE(6,26)((ET(I,J),J=1,3),I=1,7)
   26 FORMAT(1X,2HET,3E16.8)
      WRITE(6,27)((GG(I,J),J=1,3),I=1,7)
   27 FORMAT(1X,2HGG,3E16.8)
      DO 12 I=1,7
      DO 12 J=1,3
   12 ET(I,J)=GG(I,J)-ET(I,J)
      WRITE(6,26)((ET(I,J),J=1,3),I=1,7)
      DO 71 I=1,3
      DO 71 J=1,3
   71 E11(I,J)=ET(I,J)
      DO 72 I=4,7
      DO 72 J=1,3
   72 E21(I-3,J)=ET(I,J)
      CALL LSVALR(GG,N,N,M,N,ISW,WKAREA,GQ,GU,GV)
      WRITE(6,28)(GQ(I),I=1,3)
   28 FORMAT(1X,2HS,4E16.8)
      BINRM=AMAX1(1.0/GQ(1),1.0/GQ(2),1.0/GQ(3))
      CALL LSVALR(E11,N,N,M,N,ISW,WKAREA,GQ,GU,GV)
      WRITE(6,28)(GQ(I),I=1,3)
      E11NRM=AMAX1(GQ(1),GQ(2),GQ(3))
      M=4
      CALL LSVALR(E21,M,N,M   ,N,ISW,WKAREA,GQ,GU,GV)
      WRITE(6,28)(GQ(I),I=1,3)
      M=7
      E21NRM=AMAX1(GQ(1),GQ(2),GQ(3))
      ABCDEF=BINRM*E21NRM
      CHI=ABCDEF/SQRT(1.0+ABCDEF**2)
```

```
      RHS=BINRM*E11NRM+(B2NM*BINRM*CHI)/XNRM
      XRHS=BINRM*E11NRM+(BINRM**2*B2NM*E21NRM)/XNRM+BINRM**2*E21NRM**2
      WRITE(6,64)RHS,XRHS
   64 FORMAT(1X,4H RHS,E16.8,1X,5H XRHS,E16.8)
      WRITE(6,22)RHS,BINRM,E11NRM,BNRM,CHI,XNRM,E21NRM
   22 FORMAT(1X,1HW,7E16.8)
      XKAPBAR=ANRM*BINRM
      XNU=B1NRM/(ANRM*HOLD)
      WRITE(6,17)XKAPBAR,XNU
   17 FORMAT(1X,8HKAPPABAR,E16.8,3H NU,E16.8)
*
C
      DO 86 J=1,3
      H(J)=0.0
      DO 78 I=1,7
   78 H(J)=H(J)+AA(I,J)*AA(I,J)
   86 H(J)=SQRT(H(J))
      DO 80 J=1,2
      ILIM=J+1
      DO 80 I=ILIM,3
      SUM=0.0
      DO 79 K=1,7
   79 SUM=SUM+AA(K,J)*AA(K,I)
   80 CCOS(I,J)=SUM/(H(I)*H(J))
C
      M=7
      NAA=3
      NBB=1
      IAA=IBB=7
      IDGT=8
C
      CALL LLSQAR(AA,BB,M,NAA,NBB,IAA,IBB,IDGT,WKAREA,IER)
C
      WRITE(6,200)((AA(K,J),J=1,3),K=1,7)
  200 FORMAT(1H0/(1X,8HPSUEDINV,3E15.7))
      WRITE(6,100)IER
  100 FORMAT(1H0/1X,5H IER =,I10)
      WRITE(6,101)(K,BB(K),K=1,3)
  101 FORMAT(1X,3HUVW,I9,E16.8)
      SUM1=BB(1)*BB(1)+BB(2)*BB(2)+BB(3)*BB(3)
      XNRM=SQRT(SUM1)
      WRITE(6,97)SUM1,XNRM
   97 FORMAT(1H0/1X,7HUVW SQD,E16.8/1X,8HSQRT UVW,E16.8)
      DO 44 K=1,7
   44 S(K)=CC(K)-A(K)*BB(1)-B(K)*BB(2)-C(K)*BB(3)
      WRITE(6,43)(K,S(K),K=1,7)
   43 FORMAT(1H0/(1X,5HRESID,I10,E15.8))
*
      XLHS=
     1     (BB(1)-QB(1))**2+(BB(2)-QB(2))**2+(BB(3)-QB(3))**2
      WRITE(6,21)(BB(I),QB(I),I=1,3)
   21 FORMAT(1X,4HBBQB,2E16.8)
      WRITE(6,24)XLHS,HOLD
   24 FORMAT(1X,2H**,2E16.8)
      XLHS=SQRT(XLHS)/HOLD
      WRITE(6,67)XLHS,XLHS,RHS,RHS
   67 FORMAT(1X,4HXLHS,E15.8,F15.8,4H RHS,E15.8,F15.8)
```

```
*
C
      DO 75 K=1,7
   75 H(K)=SQRT(A(K)*A(K)+B(K)*B(K)+C(K)*C(K))
      DO 76 I=1,6
      JLIM=I+1
      DO 76 J=JLIM,7
      COS=(A(I)*A(J)+B(I)*B(J)+C(I)*C(J))/(H(I)*H(J))
   76 WRITE(6,77)I,J,COS
   77 FORMAT(1H0,5X,10HROW COSINE,2I3,E16.8)
      DO 81 J=1,2
      ILIM=J+1
      DO 81 I=ILIM,3
   81 WRITE(6,82)J,I,CCOS(I,J)
   82 FORMAT(1H0,5X,13HCOLUMN COSINE,2I3,E16.8)
C
      N=3
      IA=IAA
      ISW=1
      CALL LSVALR(Q,M,N,IA,IA,ISW,WKAREA,S,G,V)
      WRITE(6,88)(K,S(K),K=1,3)
   88 FORMAT(1H0/(10X,8HSING VAL,I5,E16.8))
      WRITE(6,89)((G(I,J),J=1,N),I=1,M)
   89 FORMAT(1H0/(1X,1HU,3E15.8))
      WRITE(6,90)((V(I,J),J=1,N),I=1,N)
   90 FORMAT(1H0/(1X,1HV,3E15.8))
      WRITE(6,94)((TKK(I,J),J=1,3),I=1,3)
   94 FORMAT(1H0/(1X,3HTKK,3E15.8))
      BQ(1)=BQ(2)=BQ(3)=0.0
      CALL LLSQAR(TKK,BQ,3,3,1,3,3,8,WKAREA,IER)
      WRITE(6,93)IER
   93 FORMAT(1X,5HIER =,I10)
      WRITE(6,95)((TKK(I,J),J=1,3),I=1,3)
   95 FORMAT(1H0/(1X,7HTKK PSI,3E16.8))
C
   34 CONTINUE
C
      STOP
      END
```

```
      SUBROUTINE VCOMP(V,Q,M,N)
      DIMENSION V(7,7),VA(7,7),Q(7,7),INDEX(10),INV(10),C(10)
      DIMENSION WKAREA(250)
      IF (M.GT.0) GO TO 400
      NPO=N+1
      DO 33 J=NPO,M
      DO 33 I=1,M
   33 V(I,J)=0.0
      DO 2 I=1,M
      DO 1 J=1,M
    1 VA(I,J)=0.0
    2 VA(I,I)=1.0
      DO 3 I=1,N
    3 INDEX(I)=I
      DO 50 I=1,N
      IF (V(I,I).NE.0.0) GO TO 49
      DO 80 J=I,N
      IF (V(I,J).EQ.0.0) GO TO 80
      ISTORE=INDEX(I)
      INDEX(I)=INDEX(J)
      INDEX(J)=ISTORE
      GO TO 81
   80 CONTINUE
      WRITE(6,83)
   83 FORMAT(1H1/(1X,8HNO PIVOT))
      STOP
   81 DO 82 K=1,M
      STORE=V(K,I)
      V(K,I)=V(K,J)
      V(K,J)=STORE
      STORE=VA(K,I)
      VA(K,I)=VA(K,J)
   82 VA(K,J)=STORE
   49 STORE=V(I,I)
      DO 51 J=I,N
      V(I,J)=V(I,J)/STORE
   51 VA(I,J)=VA(I,J)/STORE
      IPO=I+1
      DO 53 K=1,M
      IF (K.EQ.I) GO TO 53
      STORE=V(K,I)
      DO 54 J=I,N
      V(K,J)=V(K,J)-STORE*V(I,J)
   54 VA(K,J)=VA(K,J)-STORE*VA(I,J)
   53 CONTINUE
   50 CONTINUE
      IDGT=8
      CALL LINV2F(VA,M,M,V,IDGT,WKAREA,IER)
      WRITE(6,67)IER
   67 FORMAT(1X,3HIER,I10)
      DO 39 I=1,N
   39 INV(INDEX(I))=I
      WRITE(6,201)(INV(I),I=1,N)
  201 FORMAT(1X,3HINV,10I10)
      WRITE(6,200)(INDEX(I),I=1,N)
  200 FORMAT(1X,5HINDEX,10I10)
      DO 38 J=1,M
```

```
      DO 38 I=1,M
   38 Q(I,J)=V(I,INV(J))
  400 DO 402 J=N,M
      DO 401 I=1,M
  401 Q(I,J)=0.0
  402 Q(J,J)=1.
      DO 403 J=1,N
      DO 403 I=1,M
  403 Q(I,J)=V(I,J)
      SUM=0.0
      DO 20 I=1,M
   20 SUM=SUM+Q(I,1)**2
      SUM=SQRT(SUM)
      DO 21 I=1,M
   21 Q(I,1)=Q(I,1)/SUM
      DO 22 L=2,M
      LMO=L-1
      DO 23 K=1,LMO
      C(K)=0.0
      DO 23 I=1,M
   23 C(K)=C(K)+Q(I,L)*Q(I,K)
      DO 26 I=1,M
      DO 26 K=1,LMO
   26 Q(I,L)=Q(I,L)-C(K)*Q(I,K)
      SUM=0.0
      DO 27 I=1,M
   27 SUM=SUM+Q(I,L)**2
      SUM=SQRT(SUM)
      DO 28 I=1,M
   28 Q(I,L)=Q(I,L)/SUM
   22 CONTINUE
      DO 100 I=1,M
      DO 100 J=I,M
      SUM=0.
      DO 99 K=1,M
   99 SUM=SUM+Q(K,I)*Q(K,J)
  100 WRITE(6,101)I,J,SUM
  101 FORMAT(1X,5HIJSUM,2I5,E15.8)
      RETURN
      END
```

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